2011 INCITE Projects

at the Argonne Leadership Computing Facility

Biological Sciences

Multiscale Blood Flow Simulations
George Karniadakis, Brown University
Intrepid Allocation: 50,000,000 Hours

Protein-Ligand Interaction Simulations and Analysis
T. Andrew Binkowski, Argonne National Laboratory
Intrepid Allocation: 20,000,000 Hours

Simulation and Modeling of Membranes Interactions with Unstructured Proteins and Computational Design of Membrane Channels for Absorption of Specified Ions
Igor Tsigelny, University of California–San Diego
Intrepid Allocation: 4,000,000 Hours

Towards Breakthroughs in Protein Structure Calculation and Design
David Baker, University of Washington
Intrepid Allocation: 30,000,000 Hours

Chemistry

Simulations of Deflagration-to-Detonation Transition in Reactive Gases
Alexei Khokhlov, University of Chicago
Intrepid Allocation: 18,000,000 Hours

Potential Energy Surfaces for Simulating Complex Chemical Processes
Donald Truhlar, University of Minnesota
Intrepid Allocation: 15,000,000 Hours

Large Eddy Simulation of Two-phase Flow Combustion in Gas Turbines
Thierry Poinsot, European Center for Research and Advanced Training in Scientific Computation
Intrepid Allocation: 10,000,000 Hours

Ab Initio Dynamical Simulations for the Prediction of Bulk Properties
Theresa Windus, Iowa State University
Intrepid Allocation: 10,000,000 Hours

Computer Science

Performance Evaluation and Analysis Consortium End Station
Patrick Worley, Oak Ridge National Laboratory
Intrepid Allocation: 10,000,000 Hours

Scalable System Software for Performance and Productivity
Ewing Lusk, Argonne National Laboratory
Intrepid Allocation: 5,000,000 Hours

Trace Collection for Simulation-driven Co-design of Exascale Platforms and Codes
David Evensky, Sandia National Laboratory
Intrepid Allocation: 5,000,000 Hours

Earth Science

Climate-Science Computational Development Team: The Climate End Station II
Warren Washington, National Center for Atmospheric Research
Intrepid Allocation: 40,000,000 Hours

Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence
Susan Kurien, Los Alamos National Laboratory
Intrepid Allocation: 35,000,000 Hours

Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 4Hz
Thomas Jordan, University of Southern California
Intrepid Allocation: 10,000,000 Hours

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Energy Technologies

Advanced Reactor Thermal Hydraulic Modeling
Paul Fischer, Argonne National Laboratory
Intrepid Allocation: 25,000,000 Hours

Large Eddy Simulation for Green Energy and Propulsion Systems
Umesh Paliath, GE Global Research
Intrepid Allocation: 20,000,000 Hours

Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air
Jack Wells, Oak Ridge National Laboratory
Intrepid Allocation: 15,000,000 Hours

Engineering

Detached-Eddy Simulations and Noise Predictions for Tandem Cylinders
Philippe Spalart, Boeing
Intrepid Allocation: 45,000,000 Hours

Simulation of High Reynolds Number Turbulent Boundary Layers
Robert Moser, University of Texas at Austin
Intrepid Allocation: 40,000,000 Hours

Turbulent Multi-material Mixing in the Richtmyer-Meshkov Instability
Sanjiva Lele, Stanford University
Intrepid Allocation: 12,000,000 Hours

Uncertainty Quantification for Turbulent Mixing
James Glimm, State University of New York, Stony Brook
Intrepid Allocation: 10,000,000 Hours

Materials Science

Petascale Simulations of Stress Corrosion Cracking
Priya Vashishta, University of Southern California
Intrepid Allocation: 45,000,000 Hours

High-Fidelity Simulation of Complex Suspension Flow for Practical Rheometry
William George, National Institutes of Standards and Technology
Intrepid Allocation: 25,000,000 Hours

Probing the Non-scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations
Jeffrey Greeley, Argonne National Laboratory
Intrepid Allocation: 15,000,000 Hours

Vibrational Spectroscopy of Liquid Mixtures and Solid/Liquid Interfaces
Giulia Galli, University of California–Davis
Intrepid Allocation: 15,000,000 Hours

Physics

Study of Buoyancy-driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models
Donald Lamb, The University of Chicago
Intrepid Allocation: 80,000,000 Hours

Lattice QCD
Paul Mackenzie, Fermi National Accelerator Laboratory
Intrepid Allocation: 50,000,000 Hours

Simulations of Laser-plasma Interactions in Targets for the National Ignition Facility and Beyond
Denise Hinkel, Lawrence Livermore National Laboratory
Intrepid Allocation: 50,000,000 Hours

Nuclear Structure and Nuclear Reactions
James Vary, Iowa State University
Intrepid Allocation: 15,000,000 Hours

Advanced Simulations of Plasma Microturbulence at the Petascale and Beyond
William Tang, Princeton Plasma Physics Laboratory
Intrepid Allocation: 8,000,000 Hours

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U.S. DEPARTMENT OF ENERGY

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